Charge-spin-orbital dynamics of one-dimensional two-orbital Hubbard model

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Abstract.

We study the real-time evolution of a charge-excited state in a one-dimensional e_g-orbital degenerate Hubbard model, by a time-dependent density-matrix renormalization group method. Considering a chain along the z direction, electrons hop between adjacent $3z^2-r^2$ orbitals, while x^2-y^2 orbitals are localized. For the charge-excited state, a holon-doublon pair is introduced into the ground state at quarter filling. At initial time, there is no electron in a holon site, while a pair of electrons occupies $3z^2-r^2$ orbital in a doublon site. As the time evolves, the holon motion is governed by the nearest-neighbor hopping, but the electron pair can transfer between $3z^2-r^2$ orbital and x^2-y^2 orbital through the pair hopping in addition to the nearest-neighbor hopping. Thus holon and doublon propagate at different speed due to the pair hopping that is characteristic of multi-orbital systems.

1. Introduction

Competing interaction among charge, spin, and orbital degrees of freedom plays a crucial role in the emergence of various types of quantum phases in strongly correlated electron systems with active orbital degree of freedom [1, 2, 3]. The change of conditions, such as temperature, magnetic field, pressure, and chemical doping, gives rise to a dramatic change of transport and magnetic properties through a phase transition because of a subtle balance between multiple phases.

Recent developments in femto-second laser technology have made it possible to investigate the dynamical control of the many-body electron state on an ultrafast time scale, the so-called photo-induced phase transition [4]. In general, the photo-irradiation can excite the system to a novel non-equilibrium state that cannot be accessed by simply changing temperature, since photon energy is much higher than thermal energy. A photo-excited non-equilibrium state eventually relaxes to the original equilibrium state. However, the system exhibits a transient behavior and sometimes it decays into a metastable state rather than the original state. In $Pr_{0.7}Ca_{0.3}MnO_3$, a charge/orbital-ordered insulating state is melted and a ferromagnetic metallic state is induced by the photo-irradiation [5, 6]. Such a photo-induced insulator-to-metal transition has also been demonstrated in $Nd_{0.5}Ca_{0.5}MnO_3$ [7].

In this paper, to gain deep insight into the ultrafast non-equilibrium dynamics of the complex charge-spin-orbital state, we investigate the real-time dynamics of a charge-excited state in an e_g-orbital model from the viewpoint of the time evolution of wavepackets by exploiting numerical techniques. We discuss the effects of the pair-hopping interaction on the propagation of holon and doublon.

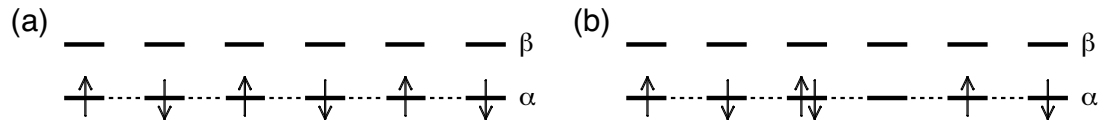

Figure 1. Electron configuration of (a) ground state and (b) charge-excited state. Dotted lines indicate hopping connection between adjacent α orbitals

2. Model and numerical method

Let us consider an $e_{\rm g}$-orbital degenerate Hubbard model on the linear chain along the z direction with N sites and one electron per site (quarter filling), described by

$$\begin{aligned} H &= \sum_{i,\tau,\tau',\sigma} t_{\tau\tau'}(d^\dagger_{i\tau\sigma}d_{i+1\tau'\sigma}+{\rm h.c.}) + U\sum_{i,\tau}\rho_{i\tau\uparrow}\rho_{i\tau\downarrow} + U'\sum_{i,\sigma,\sigma'}\rho_{i\alpha\sigma}\rho_{i\beta\sigma'} \\ &\quad + J\sum_{i,\sigma,\sigma'} d^\dagger_{i\alpha\sigma}d^\dagger_{i\beta\sigma'}d_{i\alpha\sigma'}d_{i\beta\sigma} + J'\sum_{i,\tau\neq\tau'} d^\dagger_{i\tau\uparrow}d^\dagger_{i\tau\downarrow}d_{i\tau'\downarrow}d_{i\tau'\uparrow}, \end{aligned} \tag{1}$$

where $d_{i\tau\sigma}$ is an annihilation operator for an electron with spin σ ($=\uparrow,\downarrow$) in orbital τ ($=\alpha$ for $3z^2-r^2$; β for x^2-y^2) at site i, and $\rho_{i\tau\sigma}=d^\dagger_{i\tau\sigma}d_{i\tau\sigma}$. The hopping amplitude is given by $t_{\alpha\alpha}=1$ (taken as energy unit), $t_{\alpha\beta}=t_{\beta\alpha}=t_{\beta\beta}=0$. Note that due to the orbital anisotropy, $3z^2-r^2$ orbital becomes itinerant, while x^2-y^2 orbital is localized. Regarding the on-site Coulomb interaction, U is the intra-orbital Coulomb interaction, U' the inter-orbital Coulomb interaction, J the inter-orbital exchange interaction, and J' the pair-hopping interaction between different orbitals. The relation $U=U'+J+J'$ holds due to the rotation symmetry in the local orbital space and $J=J'$ is assumed due to the reality of the orbital function [2], so that we have two independent interaction parameters. In this paper, we set $U'=10$ and study the dependence on J'. We use the unit such that $\hbar=1$, and the time is measured in units of $\hbar/t_{\alpha\alpha}$.

We investigate the dynamics of the charge-excited state from the viewpoint of the propagation of wavepackets [8]. For this purpose, we exploit density-matrix renormalization group (DMRG) techniques. First, the ground state $|\psi_0\rangle$ is obtained by an ordinary static DMRG method [9]. The finite-system algorithm is employed with the use of open boundary conditions. Then, as an initial state at time $t=0$, we prepare a charge-excited state by creating a holon-doublon pair, defined as

$$|\psi_1^{hd}\rangle = \sum_{\tau\tau'\sigma} t_{\tau\tau'}c^\dagger_{i\tau\sigma}c_{i+1\tau'\sigma}\,|\psi_0\rangle. \tag{2}$$

The time evolution of $|\psi_1^{hd}\rangle$ is computed by an adaptive time-dependent DMRG method [10, 11]. The second-order Suzuki-Trotter decomposition is used to describe the time-evolution operator as the product of local time-evolution operators with a small time step $\Delta t=0.02$. We keep up to $m=300$ states in renormalization steps, and the truncation error is kept below 10^{-7} during the time evolution.

3. Results

In Fig. 1(a), we depict the electron configuration of the ground state. Since the electron hopping connects α orbitals in adjacent sites, α orbital is singly occupied in every site so as to gain kinetic energy. Localized $S=1/2$ spins exhibit quasi-long-range antiferromagnetic order due to the antiferromagnetic exchange interaction. For the charge-excited state, a holon-doublon pair is created at the center of the chain, as shown in Fig. 1(b). We note that α orbital is doubly occupied in a doublon site.

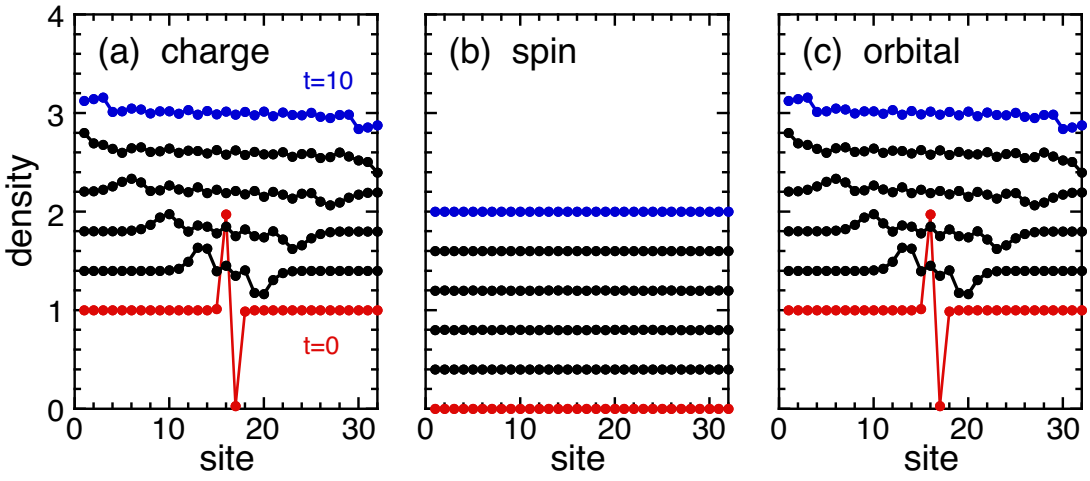

Figure 2. Time evolution of (a) charge, (b) spin, and (c) orbital densities at U'=10 and J'=0. A holon-doublon pair is introduced at the center of the chain of N=32. Time-series results from time t=0 to t=10 are arranged with shifted upward along the vertical axis.

To gain insight into the dynamics of the charge-excited state, we measure the time evolution of the charge, spin, and orbital densities, defined by $n_c(i,t)=\sum_{\tau\sigma}\langle\rho_{i\tau\sigma}\rangle_t$, $n_s(i,t)=\sum_{\tau}\langle\rho_{i\tau\uparrow}-\rho_{i\tau\downarrow}\rangle_t$, and $n_o(i,t)=\sum_{\sigma}\langle\rho_{i\alpha\sigma}-\rho_{i\beta\sigma}\rangle_t$, where $\langle\cdots\rangle_t$ denotes the expectation value using the wavefunction at time t. In Fig. 2, we present our numerical results at J'=0. Concerning the charge density, a holon-doublon pair is completely localized at the chain center at t=0, i.e., $n_c(N/2,0)\simeq 2$ and $n_c(N/2+1,0)\simeq 0$, as shown in Fig. 2(a). As the time evolves, holon and doublon wavepackets expand in the system. We see that the wavefront of the holon wavepacket propagates toward right, while that of the doublon wavepacket moves left, but there is no fine structure in the region between two wavefronts due to interference effects. Note that holon and doublon wavepackets propagate with the same speed, since holon and doublon move through the electron hopping of the same amplitude $t_{\alpha\alpha}$. On the other hand, as shown in Fig. 2(b), the spin density is not affected by the charge excitation, since we assume S^z_{tot}=0 for the charge-excited state, where S^z_{tot} is the z component of total spin. As shown in Fig. 2(c), the orbital density is equivalent to the charge density. Once two electrons occupy α orbital in the doublon site, β orbital is always vacant due to the absence of the pair-hopping process at J'=0, so that $n_c(i,t)=n_o(i,t)=\sum_{\sigma}\langle\rho_{i\alpha\sigma}\rangle_t$.

At finite J', however, a pair of electrons accommodated in α orbital can transfer to β orbital through the pair hopping, leading to a difference in the propagation of holon and doublon. In fact, we find that the doublon wavepacket propagates at half speed in comparison to the holon wavepacket, as shown in Fig. 3(a). Let us here discuss the effects of the pair hopping on the doublon propagation. Assuming that the electron pair occupies either α orbital or β orbital, the local two-electron state is described by the linear combination of $|i\alpha\uparrow\rangle|i\alpha\downarrow\rangle$ and $|i\beta\uparrow\rangle|i\beta\downarrow\rangle$, where $|i\tau\sigma\rangle=d^\dagger_{i\tau\sigma}|0\rangle$ and $|0\rangle$ is the vacuum state. With these two states, the eigenstates are given by $|ia\rangle\equiv(|i\alpha\uparrow\rangle|i\alpha\downarrow\rangle-|i\beta\uparrow\rangle|i\beta\downarrow\rangle)/\sqrt{2}$ and $|ib\rangle\equiv(|i\alpha\uparrow\rangle|i\alpha\downarrow\rangle+|i\beta\uparrow\rangle|i\beta\downarrow\rangle)/\sqrt{2}$ with its eigenenergy $E_a=U-J'$ and $E_b=U+J'$, respectively. Among them, we suppose that the lowest-energy state $|ia\rangle$ represents the doublon state in the strong-coupling limit. Then, doublon and single electron can be exchanged by an effective hopping,

$$\langle i+1\alpha\sigma'|\langle ia|t_{\alpha\alpha}(c^\dagger_{i\alpha\sigma}c_{i+1\alpha\sigma}+\text{h.c.})|i\alpha\sigma'\rangle|i+1a\rangle=-\frac{1}{2}t_{\alpha\alpha}\delta_{\sigma,-\sigma'}. \tag{3}$$

Namely, the hopping amplitude for doublon is reduced to half of the original hopping amplitude

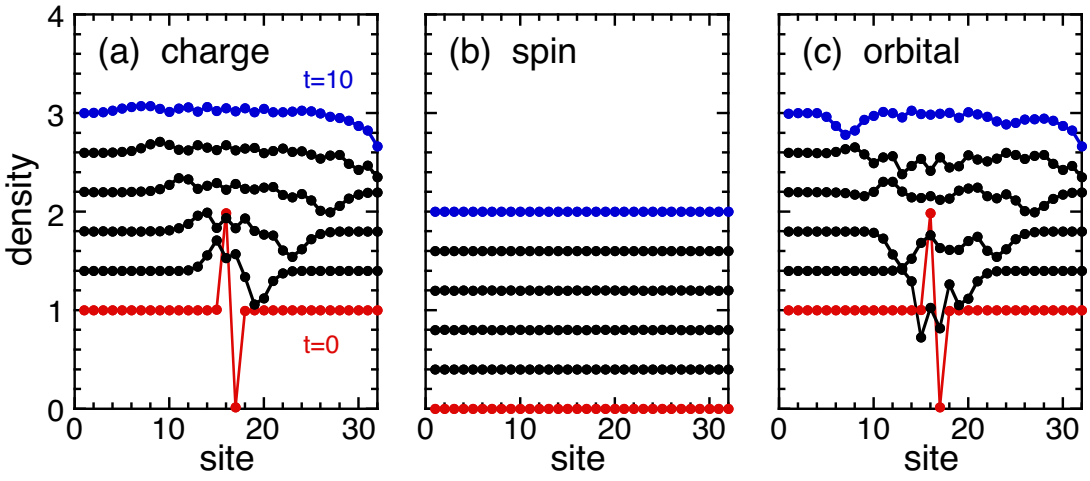

Figure 3. Time evolution of (a) charge, (b) spin, and (c) orbital densities at U'=10 and J'=2.

due to the pair hopping. On the other hand, holon and single electron are exchanged with the original hopping amplitude. Thus doublon propagates at half speed comparing with holon.

For the spin state, no structure appears in the spin density even at J'=2, as shown in Fig. 3(b). Figure. 3(c) presents the orbital density. We can see a correspondence of the orbital density to the charge density, while they are not equivalent any longer. In fact, regarding the right-moving wavefront, the orbital density is quite similar to the charge density. The left-moving wavefront of the orbital density propagates with the same speed as that of the left-moving wavefront of the charge density. However, the difference of the orbital density from the uniform value varies between positive and negative as the time evolves, indicating that the electron pair actually occupies not only α orbital but also β orbital. Thus the orbital structure around doublon is dynamically deformed due to the pair hopping.

4. Summary

We have studied the time evolution of the charge-excited state of the one-dimensional e_g-orbital degenerate Hubbard model by using DMRG techniques. We have shown that doublon propagates at half speed in comparison to the holon motion because of the pair-hopping process peculiar to multi-orbital systems.

Acknowledgments

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